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Self-tuning PID control of jacketed batch polystyrene reactor using genetic algorithm

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Abstract

Self-tuning PID controller with genetic algorithm (GA) was applied to the temperature control of a jacketed batch polymerization reactor and thus tracking performance of optimal temperature profile was investigated. To obtain optimal tuning parameters of this controller, genetic algorithm was used. The fitness function for GA was taken as the integral of the absolute value of the error (IAE). By using tuning parameters three different optimal temperature trajectories were obtained, the efficiency and the performance of the self-tuning PID controller with GA was examined by simulation and experimentally. It was observed that the control experiments were successfully conducted on tracking the optimal trajectories which would yield polymer product with desired properties. Simulation results also show that self-tuning PID control with GA give very satisfactory results.

Keywords: Polymerization reactor; Self-tuning PID control; Genetic algorithms

1. Introduction

Batch process in manufacturing of chemicals, pharmaceutical, polymers have occupied an important position in chemical industry. Batch polymerization reactions have complex mechanism, strong inherent, and nonlinearities. For this reason, the control of such polymerization reactors could be a challenging task in order to reach the desired polymer quality. Up to now, variety of control methods has been applied on chemical and polymerization reactors. Self-tuning control is a control scheme in which controller parameters are determined according to the dynamic behaviour and desired response of the process. The determination of these parameters is very important as it effects the control performance. Genetic algorithms are able to identify these parameters. GA is a different optimization method based on the mechanics of the natural genetics and natural selection [1]. It is used for nonlinear complex optimization problems. Wang and Kwok [2] used genetic algorithm for the optimization of the parameters of classical PID controllers for nonlinear processes. They compared GA with other optimization methods by giving the concept of GA and working principles. They showed that the GA could produce the smallest performance index, in comparison to the ZN and HJ methods during the same observation period. Machado and Bolzan [3] studied the control of batch suspension polymerization reactor in a pilot unit. In their study, initiator concentration and temperature were determined to produce the polymer within the desired characteristics, and a methodology was implemented to control the operation of a batch polymerization reactor by means of a self-tuning adaptive controller. Friedrich and Perne [4] showed that advanced control methods like adaptive control, self-tuning control, fuzzy and neural network controls would perform better than conventional PID control. Furthermore the desired product with minimum cost of operation and with maximum yield could be obtained by the precise control of operational conditions in chemical industry. Altınten et al. [5] have applied fuzzy control method with

Abbreviations: ARMA, autoregressive moving average; BPO, benzoylperoxide; Ga, genetic algorithm; HJ, Hooke and Jeeves; IAE, the integral of the absolute value of the error; PID, proportional-integral-derivative; STPID, self-tuning PID; ZN, Ziegler-Nichols.

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Nomenclature

A	heat transfer area of the reactor (m^2)
A_d, A_p, A_t	frequency factor for initiator decomposition, propagation and termination, respectively (s^{-1}, L/mol s, L/mol s)
C_p, C_{pc}	specific heats for the reactor content and coolant, respectively (kJ/kg K)
$e(t)$	error signal
E_d, E_p, E_t	activation energies for initiator decomposition, propagation and termination, respectively (kJ/mol K)
f	initiator efficiency
$-\Delta H$	heat of the reaction (kJ/kmol)
I, I_o	initiator concentration, initial initiator concentration (mol/L)
k_d	initiator decomposition rate constant, $2.6 \times 10^{16} \exp(-143.093/RT)$ (s^{-1})
k_p	propagation rate constant, $1.051 \times 10^7 \exp(-29.539/RT)$ (L/mol s)
k_t	termination rate constant, $1.255 \times 10^9 \exp(-7.029/RT)$ (L/mol s)
k_{tc}	termination by combination rate constant (L/mol s)
K_c	proportional gain
$\dot{m}_c$	coolant flow rate (kg/s)
M, M_o	monomer concentration, initial monomer concentration (mol/L)
M_{nd}	desired number-average molecular weight
Q	heat given from the electrical heater (kW)
r_M	reaction rate (mol/L s)
$r(t)$	set point
t, t_f	time, polymerization time (s)
T	reactor temperature (°C)
$\bar{T}_c$, T_{ci}, T_{co}	average, inlet and outlet coolant temperature (°C)
ΔT	sampling interval
$u(t)$	controller output
U	overall heat transfer coefficient (W/m^2K)
v	k_{tc}/k_t, constant
V, V_c	reactor volume, jacket volume (m^3)
X_d	desired monomer conversion
$y(t)$	process output

Greek letters

μ_r	viscosity of the reacting mixture (cp)
μ_o	zeroth moment of dead polymer distribution
$\dot{v}_c$	coolant flow rate (mL/s)
ρ	density of the reactor content (kg/m^3)
ρ_c	coolant density (kg/m^3)
τ_d	derivative time
τ_I	integral time

genetic algorithm to a polymerization reactor at a constant set point. They also examined the performance of fuzzy controller with GA in terms of its efficiency in tracking the temperature path [6]. Hapoğlu et al. [7] applied generalised minimum variance (GMV) control with genetic algorithm to a tubular flow reactor. The genetic algorithm was found very effective in determining optimal solutions to calculate model parameters. Chang et al. [8] proposed a self-tuning method for a class of nonlinear PID control systems based on Lyapunov approach. Erdoğan et al. [9] studied the optimal temperature control of batch jacketed free radical polymerization reactor with STPID control method. They used Bierman algorithm, and the control parameters were recursively identified.

In the present work, in order to find the controller parameters of self-tuning controller, a control system for a batch styrene polymerization reactor was constructed by applying genetic algorithm. The controller performance was tested by simulation and then corroborated by experiments. Optimal conditions for batch polymerization reactors were calculated to reach a desired molecular weight and conversion in minimum time by using a computer program developed for this system. The performance of self-tuning controller was examined in terms of its efficiency and duration in tracking the optimal temperature, conversion and the molecular weight changes. The results from the experiments were compared with desired and theoretical values obtained from the optimization of model equations of the polymerization reactor.

2. Optimization and reactor model

2.1. Mass balance equations

For the optimization of the batch solution polymerization process of styrene using benzoylperoxide (BPO) as the initiator, the following differential equations describe the dynamics of the reactor [10]:

Initiator:

$$\frac{d(IV)}{dt} = -k_d IV \tag{1}$$

Monomer:

$$r_M = \frac{d(MV)}{dt} = -k_p \left(\frac{2fk_d}{k_t}\right)^{1/2} MI^{1/2}V = -k_1 MI^{1/2}V \tag{2}$$

Zeroth moment of the dead polymer chains:

$$\frac{d(\mu_o V)}{dt} = 2f\left(1 - \frac{v}{2}\right)k_d IV = k_4 k_d IV \tag{3}$$

where

$$k_1 = k_p \left(\frac{2fk_d}{k_t}\right)^{1/2} = A_1 \exp\left(\frac{-E_1}{RT}\right) \tag{4}$$

$$k_4 = 2f\left(1 - \frac{v}{2}\right) \tag{5}$$

In these equations, constant density and volume, ideal mixing, quasi-steady state were assumed.

2.2. Optimization of reactor temperature trajectory

Although the molecular weight distribution of the polymer is the most important element to the properties of the product, the reaction temperature is controlled to produce a polymer which has desired properties. Temperature influences the monomer conversion and the molecular weight.

In this work, the Hamiltonian maximum principle [11] was applied to calculate the optimal temperature trajectory to reach desired properties in minimum time. The equation obtained for optimal temperature is given below:

$$T = \frac{(-E_1/R)}{\ln[E_d/(A_1 CI^{1/2}(E_1 - E_d))]} \tag{6}$$

where

$$A_1 = (2f)^{1/2} A_p A_d^{1/2} A_t^{-1/2} \tag{7}$$

$$E_1 = E_p + \frac{E_d}{2} - \frac{E_t}{2} \tag{8}$$

2.3. Energy balance equations

The energy balances for reactor and jacket can be written as follows:

$$\frac{dT}{dt} = \frac{Q}{V\rho C_p} + \frac{(-\Delta H) r_M}{\rho C_p} - \frac{UA(T - \bar{T}_c)}{V\rho C_p} \tag{9}$$

$$\frac{dT_{co}}{dt} = \frac{\dot{m}_c(T_{ci} - T_{co})}{V_c \rho_c} + \frac{UA(T - \bar{T}_c)}{V_c \rho_c C_{pc}} \tag{10}$$

For the derivation of these equations, ideal mixing, constant inlet cooling water temperature, consumption of the monomer only in the propagation state were assumed.

As the monomer conversion increases, the viscosity increases excessively. Therefore, it is important to predict the overall heat transfer coefficient as a function of viscosity of the reacting mixture as

$$U = \frac{1}{\mu_r^{0.33} S + F} \tag{11}$$

where S and F are constant which depend on the reactor size and physical properties.

3. Design of self-tuning PID control using genetic algorithm

The self-tuning PID controller with GA was depicted for the temperature control of the polymerization reactor. The performance of self-tuning PID control depends on its design parameters. In this study, genetic algorithm is utilized to find these parameters. The main basic idea in self-tuning control is to fix the controller structure by defining system dynamic and to tune to controller parameters according to the defined and desired responses of the process. Self-tuning systems generally

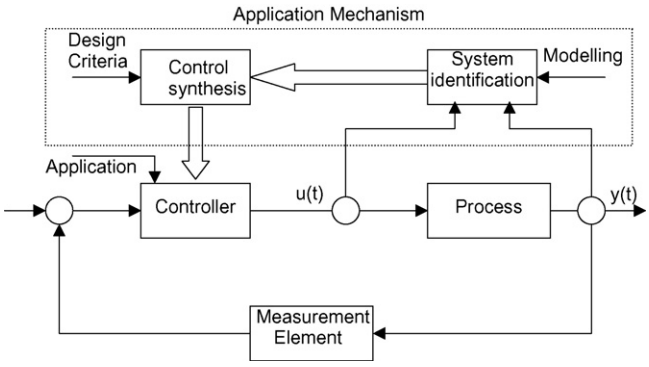

Fig. 1. Block diagram of self-tuning PID controller.

are microprocessor based systems and discrete-time modeling is convenient. The model structure is explained according to the polynomial order of the model parameters. The diagram of a self-tuning PID control system is shown in Fig. 1. Self-tuning strategy here is implemented in a feedback manner. Three sets of computations are employed: system identification, control synthesis and implementation of the settings in a feedback loop.

The control equation is given as follows

$$u(t) = \frac{S}{R}[r(t) - y(t)] \tag{12}$$

Here $r(t)$ represents the set point, and:

$$S = s_0 + s_1 z^{-1} + s_2 z^{-1}; \qquad R = 1 - z^{-1} \tag{13}$$

The system ARMA model is given as

$$y(t) = \frac{b_0 z^{-1}}{1 + a_1 z^{-1} + a_2 z^{-2}} u(t) = \frac{B}{A} u(t-1) \tag{14}$$

Transfer function of a self-tuning PID controller can be written by replacing Eq. (12) into Eq. (14) as follows

$$y(t) = \frac{b_0 z^{-1}[s_0 + s_1 z^{-1} + s_2 z^{-2}]}{(1 - z^{-1})(1 + a_1 z^{-1} + a_2 z^{-2})} r(t) = \frac{BS}{T} r(t-1) + b_0 z^{-1}(s_0 + s_1 z^{-1} + s_2 z^{-2}) \tag{15}$$

The closed-loop T polynomial can be given in the form of

$$\begin{aligned} T &= 1 + t_1 z^{-1} + t_2 z^{-2} + t_3 z^{-3} \\ &= (1 - z^{-1})(1 + a_1 z^{-1} + a_2 z^{-2}) \\ &\quad + b_0 z^{-1}(s_0 + s_1 z^{-1} + s_2 z^{-2}) \end{aligned} \tag{16}$$

where t_1, t_2, t_3, a_1, a_2 and b_0 are the tuning parameters of STPID controller.

Self-tuning PID control algorithm may be summarized as follows

1. The coefficients of polynomials are calculated from the following equations according to the tuning parameters as

$$s_0 = \frac{t_1 - a_1 + 1}{b_0} \tag{17}$$

$$s_1 = \frac{t_2 - a_2 + 1}{b_0} \tag{18}$$

$$s_2 = \frac{t_3 + a_2}{b_0} \tag{19}$$

2. The STPID control parameters are found from the values of s_0, s_1 and s_2 as

$$K_c = \frac{s_0 - s_1 - 3s_2}{2} \tag{20}$$

$$\tau_I = \frac{K_c}{K_I} = \frac{(s_0 - s_1 - 3s_2)/2}{(s_0 + s_1 + s_2)/\Delta T} \tag{21}$$

$$\tau_d = \frac{K_d}{K_c} = \frac{s_2 \Delta T}{(s_0 - s_1 - 3s_2)/2} \tag{22}$$

3. The incremental control signal Δu_n is calculated from the following equation

$$\Delta u_n = K_c \left(1 + \frac{\Delta T}{2\tau_I} + \frac{\tau_d}{\Delta T}\right) e_n + K_c \left(\frac{\Delta T}{2\tau_I} - 1 - \frac{2\tau_d}{\Delta T}\right) e_{n-1} + K_c \frac{\tau_d}{\Delta T} e_{n-2} \tag{23}$$

4. The calculated output value is compared with the set point and thus an error is found.
5. It is returned to step 3.

In this study, genetic algorithm is used to select four of the tuning parameters as a_1, a_2, b_0 and t_1. Then the algorithm of self-tuning control is implemented according to these tuning parameters. Next, the integral of the absolute value of the error (IAE) using these chosen parameter values is calculated and tuning parameters with the least error are used to control the polymerization reactor. Thus, controller parameters are tuned in such a way that the error is minimum.

4. Experimental system

Polymerization experiments were carried out in a cylindrical jacketed glass reactor of 1.1 L equipped with an impeller and electrical heater which was connected to a thyristor. In the jacket, tap water was used as a coolant. The dissolved oxygen was purged by bubbling pure nitrogen gas by means of the reaction mixture. The reactor was also equipped with a computer data acquisition and temperature control system. Fig. 2 shows the schematic of reactor set-up. Toluene, benzoylperoxide and styrene were used as solvent, initiator and monomer, respectively. After the monomer and the solvent were charged into the reactor, it was heated to the desired starting temperature then initiator BPO was added to start the polymerization. The temperature control of the reactor was carried out by using the STPID controller.

The reaction mixture was sampled at successive times. The samples were precipitated in methanol. Then, the precipitate was filtered, dried in vacuum and weighed and the monomer conversion was calculated.

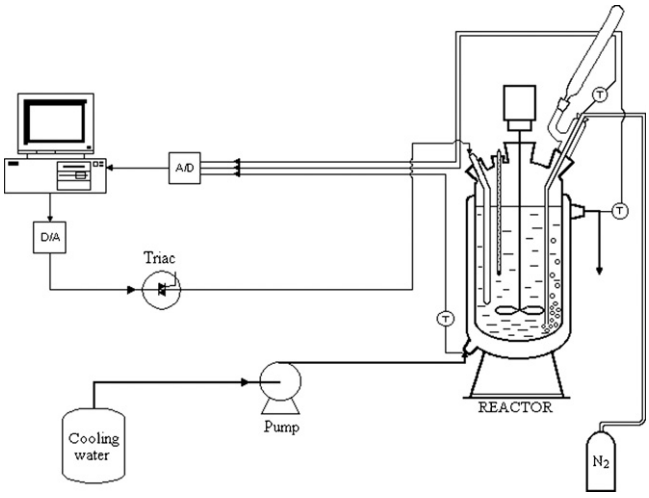

Fig. 2. Schematic diagram of the polymerization reactor control system.

5. Results and discussion

This work provides theoretical and as well as experimental study. A set of computer programs have been written to implement STPID algorithm. For the experimental studies, the VisiDAQ program developed for data acquisition and control purposes is used. In the theoretical work a computer program written in Fortran 90 is used.

In order to accomplish temperature control of the polymerization reactor by way of control parameters of STPID controller, genetic algorithm is used. GA is an optimization method based on the mechanics of natural genetics and natural selection. In this work, GA is used to select the tuning parameters (t_1, a_1, a_2, b_0) of the control system. The fitness of all individuals in the population is evaluated according to the IAE criteria. The parameters with the least error are implemented to the control system.

5.1. Influence of the genetic parameters

Genetic operators: population size (N), crossover probability (p_c), mutation probability (p_m) and maximum number of generations (M_g) were investigated before the determination of STPID control tuning parameters. The best values of these operators were chosen among the generations after a number of executions with different values of parameters [12].

5.1.1. Population size (N)

It shows the number of strings used in GA. To find the best population size, the program was evaluated for different population size values as 10-20-30-40-50 and 75. Finally, the best population size was taken as the value which gives minimum IAE at the end of maximum generation number ($M_g = 30$). The values of the parameters for this investigation are listed in Table 1. Here, the maximum generation number was fixed as 30. Figs. 3 and 4 show that the best population size is 40 at which IAE is minimum and the time to reach 6, 28 and 29 generations is minimum.

Table 1
Parameters used in the analysis of the influence of population size

Cases	p_c (%)	p_m (%)	Population size
Curve 1	60	7	10-20-30-40-50-75
Curve 2	75	3	10-20-30-40-50-75
Curve 3	85	1	10-20-30-40-50-75

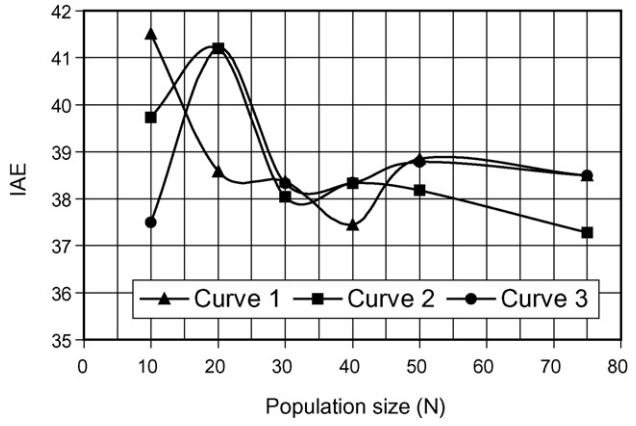

Fig. 3. The result of IAE (fitness) obtained for different population size.

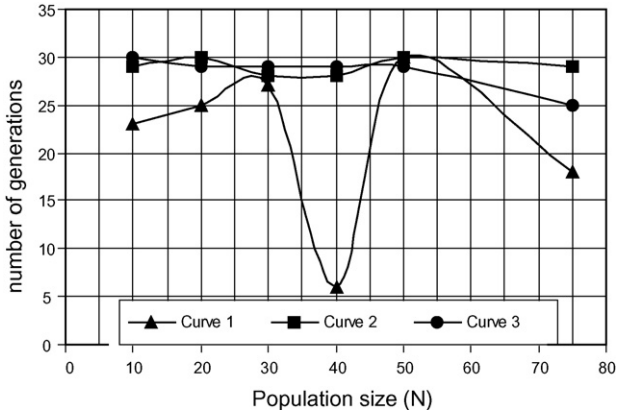

Fig. 4. The best number of generation obtained for different population size.

5.1.2. Crossover probability (p_c)

After population size is performed, crossover takes place. The computer program was run at different crossover probability values. Table 2 presents the parameters used in the analysis of the influence of the crossover probabilities. The fitness (IAE) and the number of generations obtained for these cases are shown in Figs. 5 and 6. The best result occurs with crossover probability of 0.6.

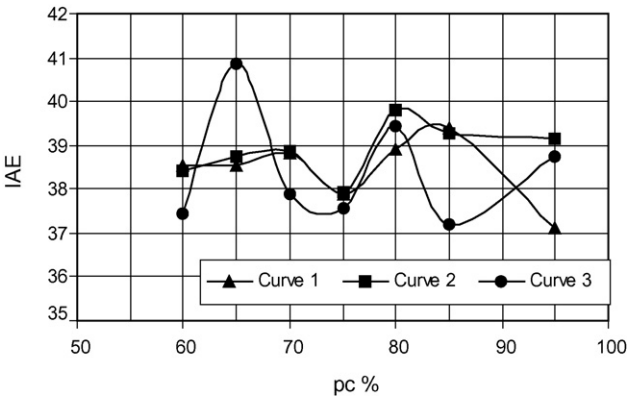

Fig. 5. The result of IAE (fitness) obtained for different crossover probability.

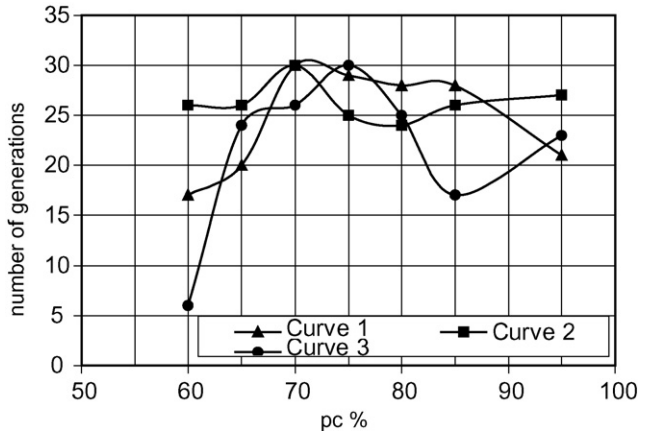

Fig. 6. The best number of generation obtained for different crossover probability.

5.1.3. Mutation probability (p_m)

Several tests with different mutation probability values (Table 3) allow to conclude that $p_m = 0.07$ is the best value. IAE values are given in Fig. 7 and number of generation is given in Fig. 8.

As a result, the optimum GA parameter values have been obtained for this control system as $N = 40$, $p_c = 60\%$ and $p_m = 7\%$. The same evaluation is performed with maximum number of generation of 50 and the same results are obtained. Maximum number of generation of 30 was chosen because of lower computational time.

5.2. Experimental work

For validation of the control strategy, the determined optimal operational conditions (Table 4) were implemented in the experimental system. Table 5 shows the steady-state

Table 2
Parameters used in the analysis of the influence of the crossover probabilities

Cases	Population size	p_m (%)	p_c (%)
Curve 1	40	4	60-65-70-75-80-85-95
Curve 2	40	5	60-65-70-75-80-85-95
Curve 3	40	7	60-65-70-75-80-85-95

Table 3
Parameters used in the analysis of the influence of the mutation probabilities

Cases	Population size	p_c (%)	p_m (%)
Curve 1	40	60	1-3-4-5-6-7-8
Curve 2	40	75	1-3-4-5-6-7-8
Curve 3	40	85	1-3-4-5-6-7-8

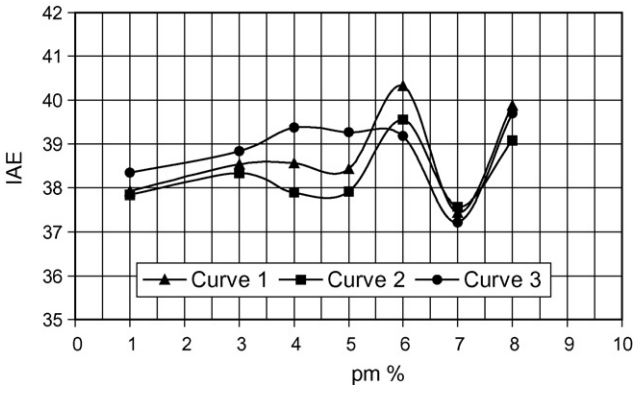

Fig. 7. The result of IAE (fitness) obtained for different mutation probability.

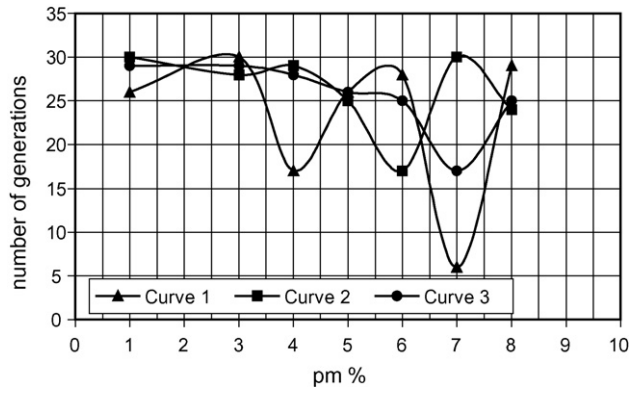

Fig. 8. The best number of generation obtained for different mutation probability.

conditions in polymerization control experiments (heater resistance = 106 Ω).

The best STPID tuning parameters were determined by the use of control parameters of GA ($N = 40$, $p_c = 60\%$, $p_m = 7\%$ and $M_g = 30$). The model parameters of the system calculated for three different optimal temperature trajectories are given in Table 6.

Then, STPID control algorithm was implemented in the experimental system to observe its efficiency. The experimental STPID control results in tracking the optimal temperature profile for three different initial initiator concentrations ($I_o = 0.0125$, 0.0150, 0.0185 mol/L) are presented in Fig. 9. Examining the profiles, it is seen that experimental profile is close to the set point path with small fluctuations for $I_o = 0.0125$ mol/L. There is a deviation (offset) from the set point in tracking the set point trajectory for $I_o = 0.0150$ mol/L. The deviation is 0.4–0.7 °C and it is mainly due to the abrupt change in the temperature trajectory at the initial part of the reaction. Later, controller shows good performance and it tracks the set point path well. A very good tracking of set point temperature path is observed for $I_o = 0.0185$ mol/L. The maximum deviation in temperature is only 0.3–0.5 °C.

Figs. 10–12 show the time variation of manipulated variable (H) that was implemented by the control system. Heat (H) was manipulated in an oscillatory manner in all cases. As it is seen in Fig. 10, the manipulated variable (H) oscillates very widely after the point at which the profile is being ramped up. The

Table 6
Tuning parameter value obtained by using GA for three different temperature paths

Run	t_1	a_1	a_2	b_0
1	−0.288235306	−0.038416423	0.251275655	0.000730132
2	−0.288235306	−0.040371457	0.247303026	0.000734968
3	−0.297647071	−0.048973608	0.252020523	0.000700630

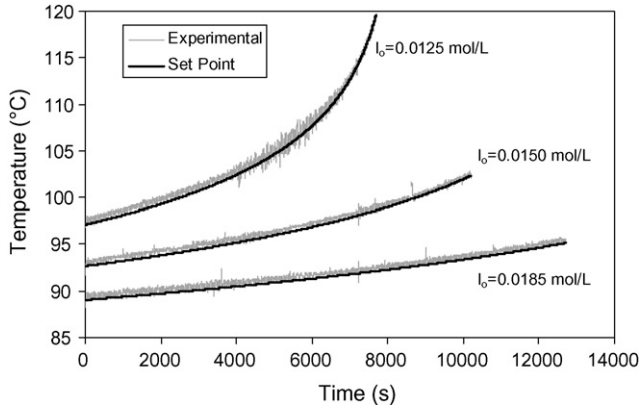

Fig. 9. STPID control results in tracking the optimal temperature profile for three different initial initiator concentrations ($I_o = 0.0125$, 0.0150, 0.0185 mol/L).

Table 4
The operating conditions

Run	M_o (mol/L)	X_d (%)	M_{nd} (g/mol)	I_o (mol/L)	$T_{R,first}$ (°C)	t_f (s)
1	6.092	50	52,000	0.0125	97.1	7,620
2	6.092	50	52,000	0.0150	92.7	10,200
3	6.092	50	52,000	0.0185	89.0	12,720

Table 5
The steady-state conditions (experimental and theoretical)

Run	$T_{reactor}$ (°C)	T_{ci} (°C)	T_{co} (°C)	$\dot{v}_c$ (mL/s)	H (experimental)	$Q(W)$ (theoretical)
1	97.1	21	79.8	0.5	80	165.11
2	92.7	21	76	0.5	75	156.75
3	89	21	73.3	0.5	70	148.40

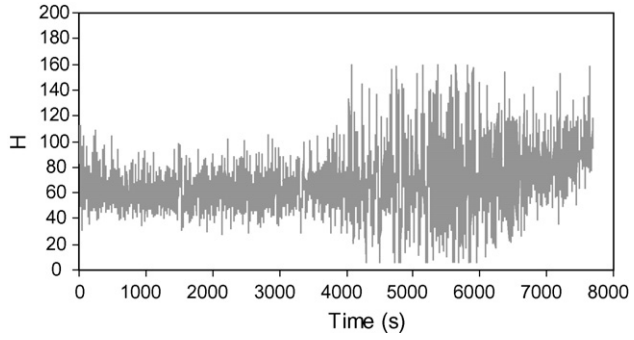

Fig. 10. Time variations of manipulated variable for the profile obtained at $I_o = 0.0125$ mol/L.

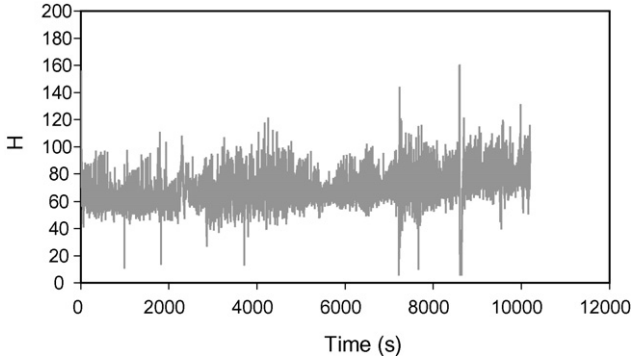

Fig. 11. Time variations of manipulated variable for the profile obtained at $I_o = 0.0150$ mol/L.

variation of H is almost the same and less aggressive in other runs. The control system is too sensitive to load disturbances that sampling from the reactor may cause the variations in reactor temperature and as a result the manipulated variable (H) acts more aggressively during the sampling. The sensitivity of the system may decrease in larger reactors.

The experimental conversion and average molecular weight values were measured by sampling successively during the experiment. The predicted and experimental results for monomer conversion at $I_o = 0.0125$ mol/L are given in Fig. 13. At the end of this experiment conversion value is 58% and the number of average molecular weight reaches its target value at 52,063 g/mol. The desired conversion values were

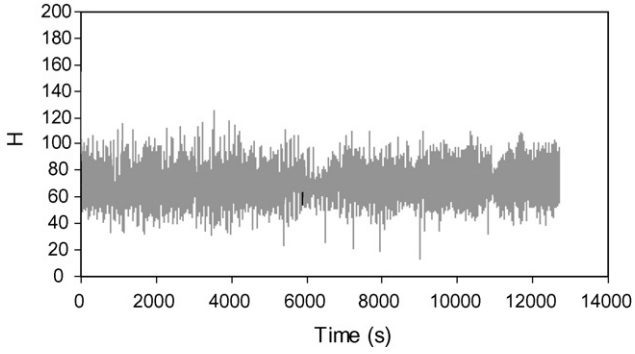

Fig. 12. Time variations of manipulated variable for the profile obtained at $I_o = 0.0185$ mol/L.

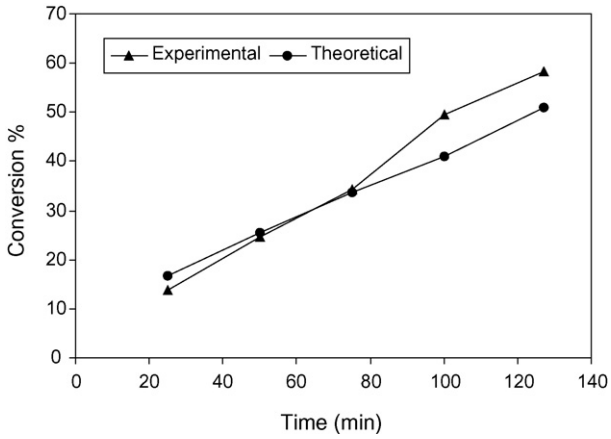

Fig. 13. Experimental and theoretical monomer conversions for the profile obtained at $I_o = 0.0125$ mol/L.

Table 7
Comparison between the measured values of M_n (g/mol)

I_o (mol/L)	0.0125	0.0150	0.0185
Control free [9]	21,000	13,900	11,800
PID [9]	36,900	48,300	46,200
STPID with GA	52,063	55,720	44,690
Desired	50,000	50,000	50,000
Error for STPID with GA	0.04126	0.1144	0.1162

achieved during the first 75 min. In the latter part, the measured values were higher than those predicted. This discrepancy may be due to the imperfect mixing of the reaction mixture and nonhomogenity as a result of significantly increased viscosity. At the end, the measured conversion is 64% and measured number of average molecular weight is 55,720 g/mol for $I_o = 0.0150$ mol/L. The experimental monomer conversion (69.4%) is higher than expected (50%), although the number of average molecular weight (44,690 g/mol) approaches its target value (50,000 g/mol) for $I_o = 0.0185$ mol/L. This error may be considered reasonable if one takes into account the analytical measurement precision. The deviations in the monomer conversions may be due to model uncertainties and unknown disturbances like the variation of heat transfer coefficient with time, solvent evaporation, volume change, and the variation of the effectiveness factor of initiator with composition. In modeling, the volume and the effectiveness factor of the initiator were taken as constant.

These experimental results mark that the best control is obtained in the first case ($I_o = 0.0125$ mol/L). Here the polymer product with desired properties is obtained in minimum time by operating the batch reactor at optimal operating conditions under STPID control with GA. Comparison between measured values of M_n at different optimal operating conditions under different controllers are given in Table 7.

6. Conclusion

The polymerization reactor used for styrene production has been successfully operated under the control of self-tuning with GA. Controller performance was studied under different opti-

mal reactor temperature trajectories. Based on the experimental results it is concluded that self-tuning control with GA performs very well at tracking the optimal temperature trajectory determined by the off-line optimization of control parameters. Self-tuning control with GA presented in this article can be extended to semi-batch and continuous polymerization systems and can be used with modifications to control the optimal temperature of an industrial polymerization reactor. This work can provide a good basis to control and operate industrial polymerization reactor.

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